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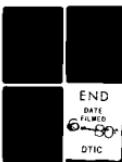
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NRL Memorandum Report 4176

Technical, Energetics, and Economic Comparison of NRL Oxidative Coal Liquefaction Process with Some Developed Coal Liquefaction Processes

R. N. HAZLETT AND J. SOLASH

*Combustion and Fuels Branch
Chemistry Division*

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) An oxidative process for the liquefaction of coal is being studied at NRL. This process offers the technical advantage of using a very common reactant, air, compared to the currently favored reductive processes (H-Coal, SRC and EDS) which require hydrogen as the reactant. The NRL process has the additional engineering advantage of operating at much lower pressures and somewhat lower temperatures than the reductive processes. The product from the NRL process is expected to have a heating value similar to that from the SRC process.			

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20. Abstract (Continued)

A net energy analysis for production of a heavy fuel oil (a potential replacement for petroleum used in large scale heating or power plants) predicts that the NRL process would have a 7 - 12 percent advantage in energy efficiency over the 69 percent efficiency of H-Coal. Further, the cost for NRL product will be 10 percent (about \$2/barrel) less than the cost of H-Coal.

Similar analyses for production of jet and diesel fuels from coal indicated a smaller advantage for the NRL process, 1 - 5 percent better than H-Coal on energy efficiency and \$1/barrel less for fuel cost.

Historically, oxidation of coal has been used to make plastic precursors or to obtain information about coal structure. In both cases very strong and uncontrollable oxidants are used and much heating value is lost or low yields of products are obtained. Hence, a reflexive negative reaction by those working in coal conversion processes is the typical response when the terms coal and oxidation are used in the context of fuel production. The NRL process, which uses low temperature, controlled, limited air oxidation, should surmount the negative image normally associated with the oxidation of coal.

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TECHNICAL, ENERGETICS, AND ECONOMIC COMPARISON
OF NRL OXIDATIVE COAL LIQUEFACTION PROCESS
WITH SOME DEVELOPED COAL LIQUEFACTION PROCESSES

I. Introduction

The production, utilization and conservation of energy is more than just of academic interest. In the Navy, the effects of rising fuel prices have been keenly felt. Prior to the oil embargo, the 1973 Navy fuel bill was \$500 million for 90 million barrels of oil equivalent (BOE) (1). By 1977 the Navy had reduced fuel usage to 60 million BOE but the costs rose to \$1.0 billion (2). Projections of the future Navy show that surface vessels and aircraft will be dependent on liquid hydrocarbon fuels well beyond the year 2000 (2). This means a secure supply of liquid fuel is and will continue to be imperative. As a consequence, NRL is conducting a fundamental research effort which aims at the liquefaction of coal by a novel air oxidation method.

In this report we will make a comparison of the NRL oxidative coal liquefaction method with some other well known coal liquefaction methods.

In the first section a technical comparison between the various liquefaction methods will be made. In sections II and III, comparisons will be made on the basis of energy efficiency and process economics respectively.

The coal conversion methods which will be considered for comparison are the following: NRL Oxidative Method (developed by NRL); H-Coal Process (developed by Hydrocarbon Research, Inc., Lawrenceville, N. J.); EDS - EXXON Donor Solvent (developed by EXXON Res. & Eng., Baytown Tx.); SRC process - Solvent Refined Coal (developed by Gulf Oil Corp, Harmarville, Pa.); Fischer-Tropsch method (FT); and a Mobil modification of the Fischer-Tropsch process to make gasoline. Tables IA & IB outline a synopsis of these different methods. The H-Coal, EDS, and SRC processes are similar in that they use the reducing agent, hydrogen, to attack the coal. Hence they are called reductive liquefaction processes.

The technical, net energy, and cost comparisons will be made on the basis of obtaining a similar product from all processes except the Fischer-Tropsch. This common product

Note: Manuscript submitted December 20, 1979.

TABLE IA

Process Descriptions of Oxidative and Reductive Coal Liquefaction Methods

Characteristics	Oxidative		Reductive		Fischer-Tropsch Mobil	
	NRL	H-Coal	EDS	SRC	Fischer-Tropsch	
Status	Lab (1-25g/day)	600 tons/day	250 tons/day	50 tons/day	Commercial	100 lbs/day
R&D Funding, \$10 ⁶ /yr	0.14	50	40	6	Operational	N.A.
Reagents	Air/Pyridine	H ₂ /Donor Solvent	H ₂ /Donor Solvent	Oxygen/H ₂ O	Oxygen/H ₂ O	Oxygen/H ₂ O
Catalyst	None required	In Reactor	Outside Reactor	None	a - Shift Reaction b - Liquid Synthesis	a - Shift reaction b - Methanol production c - Methanol → gasoline
Temperatures	Step I: <150°C Step II: 350-425°C	450-475°C	450-475°C	450-475°C	>1100°C	>1100°C
Pressures	Step I: 1 atm Step II: 5-40 atm	205 atm	135 atm	120-130 atm	20-30 atm	20-30 atm
Initiation Date	1976	1963*	1966*	1962*	1930's*	1974
Hydrogen Added, wt%	~ 0.2%	4-5%	3-4%	2-4%	~9%	8%
Chemistry	Selective, controlled oxidative and C-S bonds followed by quenching of cleavage between radicals with H atoms aromatic ring systems; possible oxidative removal of S as SO ₂	Non-selective thermal destruction of C-C 'molecule' to carbon monoxide and water; catalytic shift of CO/H ₂ ratio; catalyzed synthesis of fuels from CO and H ₂	Complete destruction of coal structure of coal to carbon monoxide and water; catalytic shift of CO/H ₂ ratio; catalyzed synthesis of fuels from CO and H ₂	Complete destruction of coal structure of coal to carbon monoxide and water; catalytic shift of CO/H ₂ ratio; catalyzed synthesis of fuels from CO and H ₂	Complete destruction of coal structure of coal to carbon monoxide and water; catalytic shift of CO/H ₂ ratio; catalyzed synthesis of fuels from CO and H ₂	Complete destruction of coal structure of coal to carbon monoxide and water; catalytic shift of CO/H ₂ ratio; catalyzed synthesis of fuels from CO and H ₂

* - Based on extensive German developmental and industrial experience in 1930's and 1940's plus U.S. developments in late 1940's and early 1950's; no current U.S. process development of Fischer-Tropsch.

TABLE 1B
Technical Issues

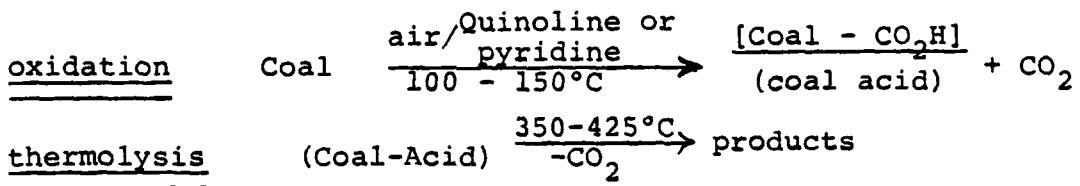
Process	Strengths	Weaknesses*
Fischer-Tropsch	Operating plant in S. Africa; major products are fuels; Mobil process permits high octane gasoline.	Approx. 50% of carbon lost as CO ₂ ; severe operating conditions and need for oxygen; long catalyst life important; most expensive method.
SRC	Simple in overall operation; no need for external catalyst (SRC-II); lower molecular weight liquids accessible by increasing temperature. High fuel gas make.	High consumption of H ₂ (SRC-II) necessary for lower MW liquid product; effect of coal derived minerals, which are used as catalysts, is uncertain; high pressure; product high in nitrogen.
EDS	Similar to SRC; Exxon Flexicoker very efficient.	High consumption of hydrogen; moderately high molecular weight products formed; catalytic hydrogenation of recycle solvent subject to deactivation by impurities; high pressure; product high in nitrogen.
H-Coal	Catalyst in reactor probably activates H ₂ addition to radicals; relatively low MW liquid product.	Very high hydrogen consumption; long catalyst life very important; high pressure operation; product high in nitrogen.
NRL	Cheap reagents (air); low temperature/pressure in oxidation step; moderate temperature/low pressure in thermal step; very low molecular weight products; relatively little gas produced.	Loss of even small amounts of process solvent raises costs.

* - Fischer-Tropsch is only process giving transportation fuels; other processes yield products which are low in hydrogen and must be further hydroreated to afford jet and diesel fuels; the hydrogen requirements for the oxidative and reductive processes will be discussed in conjunction with Table II.

for the reductive and NRL oxidative processes is a distillable fuel oil. Such an oil can be used directly for many purposes. Major uses would be for industrial heating, electric power generation, and institutional steam generation. Satisfaction of these fuel needs by coal liquids would free heavy fuel oils from petroleum for the production of transportation fuels.

Discussion, where appropriate, will address the conversion of these oils to middle distillate fuels similar to those used to power Navy ships and aircraft. This conversion has received little attention and no definitive studies have been completed.

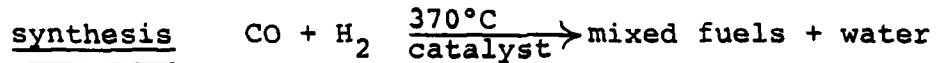
The NRL oxidative method utilizes inert polar solvents, pyridine or quinoline, to suspend or dissolve coal while air is passed through the suspension at temperatures ranging between 100 - 150°C (3,4). The oxidized coal, still in solvent suspension, is then heated to effect selective molecular decomposition. Based upon work performed at NRL the mechanism for the overall chemical transformation can be described as follows:



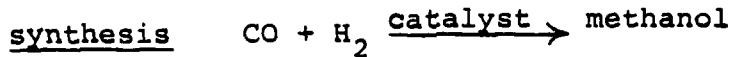
Although the temperature required for the heating step is high, catalytic techniques could lower the requirement to 250-300°C. The products found from subjecting SRC to this two-step oxidation/thermolysis sequence are highly aromatic phenanthrene-like compounds (see Appendix I for examples of chemical structures).

The Fischer-Tropsch method involves a nearly complete destruction of the coal molecule, by way of steam reforming or partial oxidation at ~1100°C, to give hydrogen, CO and much CO₂ (5). The CO/H₂ ratio is then catalytically shifted by the water-gas reaction at 340°C. Finally the CO/H₂ mixture reacts over a catalyst at 370°C to yield a wide range of products. A modified version of Fischer-Tropsch is being studied by Mobil Oil Co. The Mobil process uses the first two steps - gasification and water gas shift - of the

Fischer-Tropsch. The CO/H₂ mixture is converted catalytically to methanol which in turn reacts over a zeolite catalyst to make gasoline (6). Fischer-Tropsch chemistry is summarized by the following reactions:



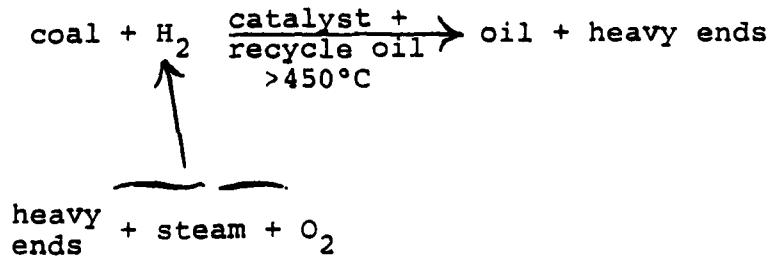
In the Mobil variation of Fischer-Tropsch, the synthesis step becomes two processes.



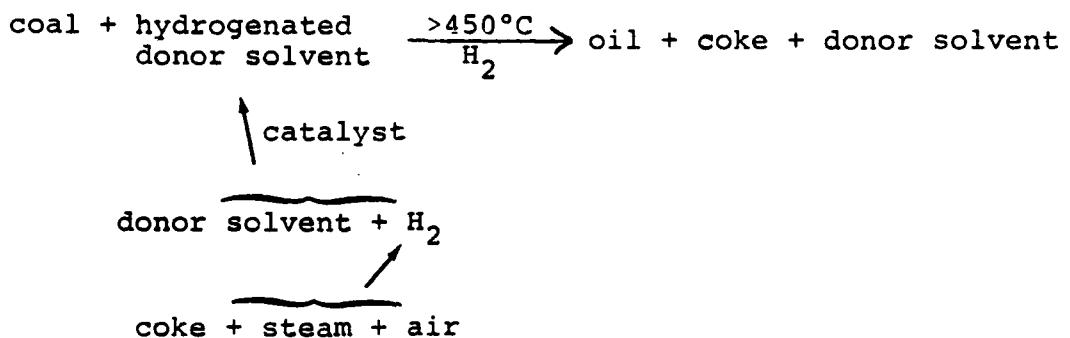
Wiser states that Fischer-Tropsch is economically unattractive in the U. S. since caking coals, which are common in the U. S., are difficult to gasify (7).

In the H-Coal process, coal is powdered, dried, and suspended or slurried in a solvent which is obtained as a product of the process (recycle oil). The coal-oil slurry is then injected into a high pressure - high temperature reaction where it comes in contact with a bed of catalyst and hydrogen (8).

Reactor temperatures are in the range 450 - 460°C at 3000 psi H₂ pressure. The product is separated by distillation (200 - 510°C) with part of the product oil being used as the solvent for the process. A scheme describing the process is as follows:

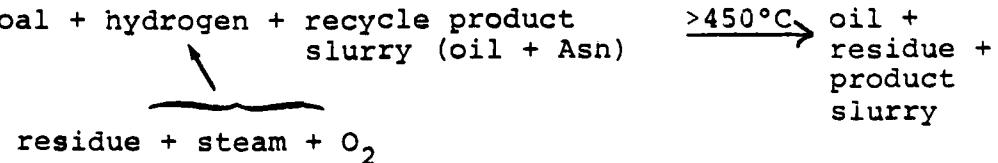


The EDS (EXXON Donor Solvent) and SRC I - II (Solvent Refined Coal) processes are quite similar in overall operation. Coal is crushed, dried and slurried in a solvent which is derived from the product oils. The slurry is then pumped into a reactor under hydrogen pressure (~2000 psi) and heated to 450°C. The product oil is distilled and the residue is coked or partially combusted. Part of the product oil is used as solvent for the process with the remainder going to market. In the EDS process, the recycle solvent is catalytically hydrotreated prior to mixing with fresh coal in a separate step. The basic chemistry of this process (EDS) is illustrated as follows (9):



The SRC I & II processes utilize the catalytic action of the coal ash to effect the hydrogenation of the recycle solvent. SRC I, a version of solvent refining, makes a low ash, low sulfur solid which has a melting point of 180°C (10, 11). This process requires a hot filtration step to remove the ash. The filtration process has encountered difficulty and more filter development is necessary to insure process reliability.

Compared to SRC-I, the SRC-II process operates at somewhat more severe conditions (longer residence time in reactor), consumes more hydrogen, but produces a liquid product (10,11). The liquid product of SRC-II is of significantly lower MW (~250-450) than SRC-I but still appreciably higher in MW than Navy fuels (MW ~100-275). The SRC-II process is summarized by the following reactions:



The H-Coal, EDS, and SRC processes effect breakdown of the coal "molecule" by severe pyrolysis of C-C and C-S bonds at elevated temperatures ($>450^{\circ}\text{C}$) (7). The radicals produced during pyrolysis may be quenched by hydrogen addition from the gas (activated by catalyst as in H-Coal process) or by hydrogen addition from the recycle solvent (as in EDS or SRC processes). Alternatively, the active radicals may be quenched by hydrogen transfer from other coal molecules. The latter coal molecules rapidly become hydrogen deficient, highly unreactive (coke) and ultimately must be partially combusted or steam reformed under severe conditions in order to be used.

The chemistry of the thermolysis step in the NRL process is different from that of the reductive processes. The oxidized coal ruptures at a lower temperature since carbon-carbon bonds are weakened by adjacent partially oxidized groups. Further, the removal of the carboxyl group, the likely oxidized function, is subject to catalysis. Thus, the NRL method has a potential for operation at a much lower temperature, $250\text{-}300^{\circ}\text{C}$, than the reductive processes.

Table II compares the yield (12), composition, and estimated heating value for products from the NRL process and two variations of the SRC process. Yield data on EDS and H-Coal can also be found in reference (12). The NRL product compares well with the SRC-I and SRC-II products in terms of yield and estimated heating value. The main product in the SRC-I process is called SRC and requires an addition of 2.5 % hydrogen to produce. The main product from the SRC-II process is a heavy oil (equivalent to a heavy fuel oil) and requires an addition of 3.5% hydrogen. The oxygen and sulfur contents of both SRC and the heavy oil are significantly reduced compared to the starting coal. In fact, twenty five percent of the hydrogen used in this liquefaction process goes into the formation of water and hydrogen sulfide. Nitrogen in coal is not significantly removed by reductive processes and conversion of coal oils to satisfactory middle distillate fuels may be severely hampered by the nitrogen problem.

TABLE II
Product Comparison Between Coal and Derived Liquid Products

Process	Product	Yield	MW	Elemental Analysis				O % (by diff.)	Heating Value BTU/lb
				C %	H %	N %	S %		
-	Raw Coal ^A	-	>1,000	71.9	5.1	1.2	3.2	9.6	13,000 ^D
SRC-I	Fuel Oil	68 ^B	~150-300	-	-	-	-	-	
	SRC	448 ^B	600	87.5	5.6	2	0.6	4	16,000 ^D
SRC-II	Naphtha	68 ^B	~70-170	-	-	-	-	-	
	Heavy Oil	338 ^B	~250-450	87.5	8.0	1.2	0.3	3	17,500 ^D
	Fuel Gas	58 ^B	-	-	-	-	-	-	
NRL	Light Oil	~30-40% ^C	~90-210	~90	~6	?	?	4?	16,500 ^D
	Residue	Unknown ^C	Unknown	-	-	-	-	-	
	Fuel Gas	< 2% ^C	-	-	-	-	-	-	

A - 9% ash
B - Flow reactor, data on yields from reference (12); data on analysis from references (11) and (13).

C - Batch reactor
D - Calculation based on elemental composition

The product from the NRL oxidative process has not been well characterized since experimental work has been restricted to a small scale. However, equipment for a 100-fold scale-up has been received, assembled, and is being applied to the problem in FY 1980. The product from this reactor will be sufficient for a detailed characterization. The nitrogen, sulfur, and oxygen content will be important criteria to define the usefulness of the NRL product as a fuel oil and as a material for conversion to middle distillate fuels.

The heat of combustion is an important property for any heating oil or fuel. Hydrogen content, and carbon content to a lesser extent, control the heating value. Thus, the liquid products from all coal liquefaction processes have significantly higher heats of combustion than the starting material. The products possess lower heat contents than typical Navy fuels, however, which currently contain hydrogen contents in the 12.5 to 14 percent range. Trends in fuel composition indicate the hydrogen content will decrease, possibly to the 11.5-13 percent range, within the next 10 years.

Therefore, the conversion of coal liquefaction products to Navy fuels would require refining to boost the hydrogen content 5-7 percent. This hydrotreatment could be accomplished at 50-90 atmospheres pressure, somewhat lower than the 120-205 atmospheres required for reductive liquefaction processes. The ease of the coal-oil to fuel conversion depends significantly on the hetero atom content of the starting material. Characterization of the NRL product from the larger scale experiments will determine whether the NRL product can be converted to a fuel more easily than the other products.

Coal liquefied by the SRC-II process takes four percent hydrogen whereas the NRL process requires 0.2 percent. Conversion of SRC-II heavy oil to a jet fuel with 13 percent hydrogen requires the addition of 5% hydrogen. On the other hand, the same conversion of NRL coal liquid to a jet fuel would require 7% hydrogen addition. Going all the way from coal to a jet fuel via SRC-II requires 9 (4+5) percent hydrogen and the NRL process needs 7.2 (0.2 + 7) percent. The major difference is due to the fact that some hydrogen in the reductive processes is sunk into lowering the oxygen and sulfur content.

The NRL oxidative liquefaction method has some clear advantages over the reductive and Fischer-Tropsch methods. The oxidation step is performed under extremely mild and controlled conditions where only 1 - 3% of the available carbon is attacked. The thermal step requires only minimal amounts of hydrogen and can even be performed in the absence of hydrogen at mild pressures and 400°C (catalysts offer the potential of lowering the thermal decomposition step temperature to 250-300°C). The complexity for the NRL process (lower temperatures and pressures) would be significantly less than for the other processes. Since hydrogen utilization during coal liquefaction is a major expense (see sections II and III) the NRL method represents a real advance over other methods.

There are some disadvantages to the NRL method. The solvents used, especially pyridine, are foul smelling, toxic, and expensive. Pyridine should be easily recoverable by distillation. However, during the thermal step we have noticed some involvement of the pyridine in the chemical breakdown of the coal. Included among the ways to suppress solvent participation are the use of a special copper catalyst (which permits lower temperature pyrolysis) and the inclusion of a very good hydrogen donor in small quantities during the thermal step.

Recent work has shown that many sulfur compounds oxidize readily under conditions which are quite similar to those used in the NRL process. Included are pyritic as well as organic forms such as dibenzthiophene (see Appendix II). The oxidized pyrites are removed as soluble salts (Meyers process) while sulfur removal from oxidized organic forms sometimes requires heating to temperature of about 300°C. It therefore seems likely that the two-step NRL process would effect some desulfurization of the coal which is processed. This point is now under investigation since sulfur removal from fuels and chars is important from an environmental as well as a product quality viewpoint.

II. Net Energy Analysis

An important aspect of energy conversion technology is the thermal efficiency of a process. Many papers have addressed this topic over the years but the most extensive and internally consistent treatment of thermal efficiency was presented by the Colorado Energy Research Institute in

1976. This group termed their approach the Net Energy Analysis and applied their analysis to a wide variety of fossil fuel conversion processes (14).

Net Energy Analysis compares the energy content of the products from a conversion process with the energy content of the input raw fossil fuel source. The analysis can be adapted for different situations but, for valid comparisons between processes, must be set up to include the same functions. For the purpose of this memorandum, the energy analysis will cover the functions of coal mining and liquefaction at a plant located adjacent to the mine site. Energy inputs include the primary source (coal) and external inputs such as fuel and electricity for operating machinery used in the process and indirect energy inputs for materials of construction, catalysts, chemicals and other features.

Thus, Net Energy Analysis as applied here takes into account energy which is used in plant construction, materials fabrication, mining, crushing, heating, compressing and pumping. Further, primary input material which is diverted to other uses such as steam generation or hydrogen production is considered in the analysis as are physical losses of material and energy.

It must be noted that while the thermal efficiencies cited below are not high in an absolute sense, energy is still being produced. The discussion centers about the questions of how much energy can be extracted from a previously unused resource and the costs involved.

An example of the application of Net Energy Analysis to a reductive coal liquefaction process is illustrated in the following Table. This analysis is for the H-Coal process operating in the synthetic crude oil mode.

TABLE III
Summary of Energy Balances for H-Coal Liquefaction Process
For Synthetic Crude Product (14)

<u>Liquefaction Energy Factors</u>	<u>% of Input Energy Used in Process</u>
Plant Materials (reactors; piping; catalysts; etc.)	2
Plant Fuels/Electricity (mining; crushing; pumping; etc.)	3
Process Consumption of Energy (process heat; H ₂ generation; compression; etc.)	19
Process Physical Loss (spills; vents; heat losses; etc.)	7
Total Process Energy Losses	31
Net Energy in Products (Thermal Efficiency)	<u>69</u>

The example demonstrates that certain process losses are quite small. For instance, "plant materials" and "plant fuels" categories combined total less than 5% of the energy losses. Clearly, the energy consumed in the process (19%) is the overriding factor in establishing the net energy for this fossil fuel conversion process. The fourth factor, physical losses, (i.e., waste heat losses), would be similar for all coal liquefaction processes. Therefore, process improvements in coal liquefaction should focus on the process consumption category where large gains are likely to be made.

A second recent evaluation of thermal efficiency of coal liquefaction has been made by K. A. Rogers and R. F. Hill of The Engineering Societies Commission on Energy (12). The efficiencies for the important conversion processes, which are tabulated in the following Table, indicate one reason why the reductive technologies (H-Coal, EDS, SRC) are favored over Fischer-Tropsch processes. Based only on thermal efficiency, the SRC processes would be selected for development.

TABLE IV

<u>Process</u>	<u>Efficiency (%)</u>
H-Coal (Syncrude)	69
EDS	64
SRC-I	70
SRC-II	70
Fischer-Tropsch	48
Fischer-Tropsch (Mobil Gasoline)	52

A major portion of the energy consumed in a reductive coal liquefaction process is related to the requirement for hydrogen. Hydrogen may be produced from external material such as natural gas or naphtha or from the input coal by steam reforming or partial oxidation. In either case, the energy loss for hydrogen production is significant, about 12% for H-Coal.

In addition to the energy lost due to hydrogen production, hydrogen compression is a major energy sink. Estimates indicate 2 to 4% of the input energy is required for hydrogen compression. We thus see that energy losses related to hydrogen utilization for the H-coal process are in the range of 14-16%.

The NRL oxidative liquefaction process uses about 1/20 of the hydrogen used in the H-Coal process. We have used hydrogen gas to blanket the oxidized coal during the thermal step (2nd step) of the NRL process (4). The hydrogen limits side reactions by trapping free radicals. Further, the hydrogen is used at a lower pressure than the pressures required in the reductive processes. Therefore, the energy loss related to hydrogen usage in the NRL scheme should be 12 to 14% less than that for the H-Coal process (on a total energy input basis). (See Appendix III for detailed calculation).

Other aspects of the NRL oxidative process reduce the thermal efficiency advantage. The main factor is associated with the oxidation step. Although the oxidation process is controlled and limited, 1 - 3% of the coal is

sacrificed in this reaction and this can be directly translated into an equivalent loss in thermal efficiency.

A second aspect relates to the use of a more expensive solvent in the NRL process compared to the reductive processes. The NRL process requires a solvent which swells coal but does not react with oxygen. The best solvent, pyridine, is an expensive, low boiling amine which is easily recoverable by distillation. Allowing for 1.0% solvent loss (with respect to product yield), the energy loss would be between one and two percent.

Summing the energy losses for oxidation and solvent, we obtain a total of 2 - 5% for the NRL process. The net difference in thermal efficiency then favors the NRL process over the H-Coal conversion process by 7 - 12% on a total energy input basis.

<p>Energy savings (NRL vs H-Coal)</p>	<p>Energy savings on hydrogen</p>	<p>Energy losses for oxidation and solvent</p>
+ 7 to 12%	= + 14 (12)%	- 2 (5)%

If the comparison between H-Coal and NRL processes are made on the basis of conversion to jet or diesel fuels, the energy savings for the NRL process would be less. However, our estimates indicate a 1 - 5 percent advantage to the NRL process on this basis.

III Economic Considerations

Recent estimates of prices for fuel oil made by conversion processes in the pilot plant stage exhibit extremely wide variations. For instance, three different calculations made in 1978-9 just for H-Coal product varied from a low of \$18 to a high of \$30 per barrel of oil (12,15,16). This suggests that cost analysis, even at the 250 ton/day pilot plant level, is extremely difficult.

The Engineering Societies Commission on Energy (ESCOE) has examined the economics of coal conversion technologies in several recent reports (12,17,18). In their report on Guidelines for Economic Evaluation (18), ESCOE presents the requirements for estimating the cost of products from a variety of conversion processes. They point out that economic estimates have large uncertainties, even those for technologies which have been operated in pilot and demonstration plants. Order of magnitude estimates for processes at the concept stage (bench level) of development would have even larger error ranges, probably of the order of 30 to 50%.

Therefore, the best approach to evaluate the price of product from the NRL process which is still at the bench level is to examine the significant differences between this process and the reductive processes.

One comparison can be made on the basis of energy losses. The previous section observed that the H-Coal process suffered an energy loss of 31% (thermal efficiency of 69% implies an overall process energy loss of 31%). Further, we found that the NRL process would have a 7 - 12% better thermal efficiency in comparison to the H-Coal process. On this basis, the energy loss for the oxidative approach would be 19 - 24%. Using a simple efficiency ratio, the price of the NRL product could be as low as $\frac{69}{81}$ (~0.85) that of the H-Coal product. Using a value of \$24 per barrel for H-Coal product, we calculate a price range of \$20 - 22 per barrel for NRL product.

A second approach considers the difference in cost of hydrogen and solvent between the two processes. H-Coal requires 2300 cu. ft. of H₂/barrel but the NRL process uses only 100 cu. ft./barrel. At \$2.50 per thousand cu.ft. for the cost of hydrogen, the H-Coal process costs \$5.50 more per barrel.

On the other hand, pyridine solvent would increase the cost of the NRL process compared to H-Coal. Allowing a loss of pyridine equivalent to 1% of the product yield, the cost for solvent (\$1.50/lb) in the NRL process would be \$3.50/barrel.

Combining the hydrogen and solvent calculations, the NRL process prices out at about \$2 less per barrel than the H-Coal process. This demonstrates the strong influence of hydrogen requirements on the price of coal liquids.

These two methods of product price comparison indicate the NRL liquefaction method would have an economic advantage over the H-Coal process of \$2 - \$4/barrel. Although a precise price cannot be assigned to products from any of the other processes, the NRL process should exhibit a similar advantage over other reductive technologies such as SRC and EDS. According to an ESCOE report, the Fischer-Tropsch processes yield products costing \$7 - \$9 more per barrel than H-Coal syncrude (12).

If the comparison between H-Coal and NRL processes are made on the basis of conversion to jet or diesel fuels, the cost of the final products would be similar. Our subjective estimates indicate a \$1 per barrel advantage to the NRL process for the coal to jet fuel case.

The NRL process has distinct engineering advantages over the reductive processes. These are associated with the lower pressure (5-40 v.s. 120 -205 atm) and temperature (400 v.s. 450°C) of the reactor. Further, the NRL process has the potential via catalysts of a much lower temperature requirement. Although these parameters do not have a large cost impact over a 20 year amortization schedule, one or more years could be saved in the fabrication of reactor vessels for the milder conditions. Process downtime would be less for the NRL process also.

In conclusion, the NRL process offers a decided advantage over the other processes and there are still some very promising leads for considerable improvement.

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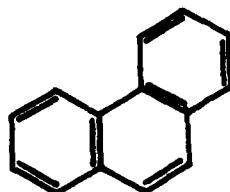
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APPENDIX I

I.A. Examples of products found from SRC after NRL two-step treatment:

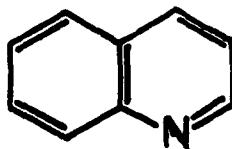


Fluorene

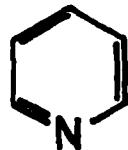


Phenanthrene

I.B. Solvents used in the NRL process:

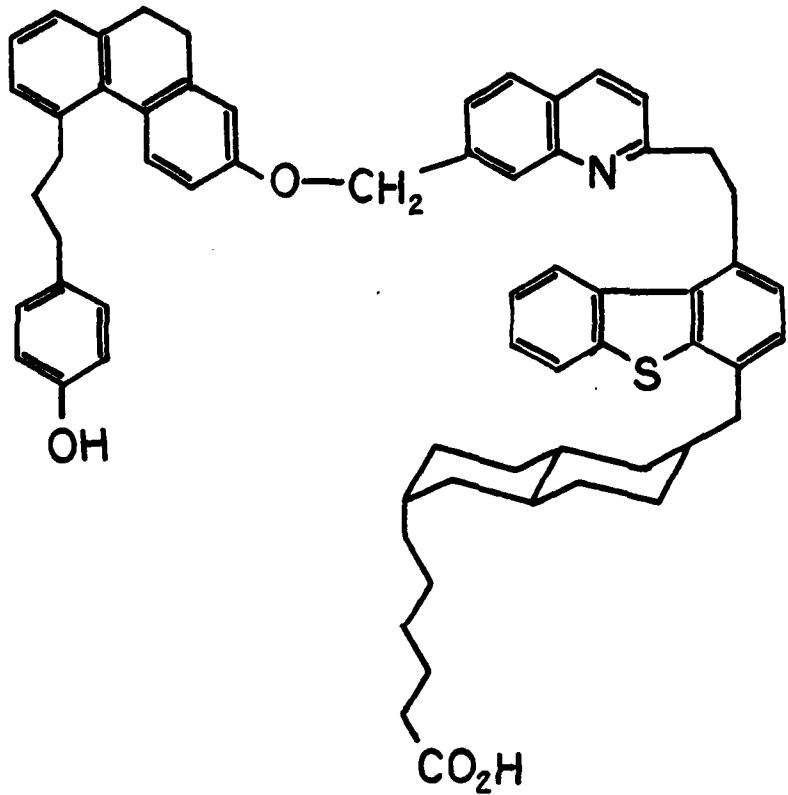


Quinoline



Pyridine

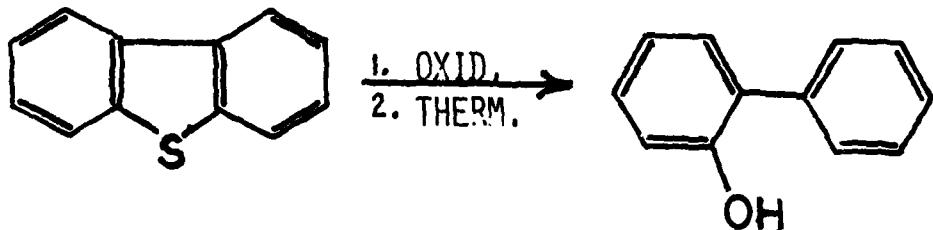
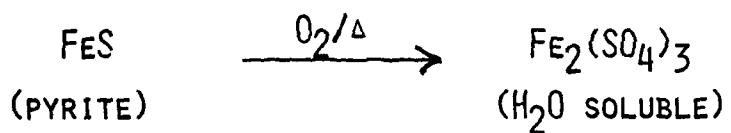
I.C. Possible partial structure of a coal "Molecule":



This structure illustrates the main types of linkage between ring clusters and also some of the heteroatom forms that are found in coal.

APPENDIX II

Behavior of sulfur forms during oxidation and thermolysis:

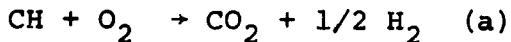


APPENDIX III

Detailed Estimate of Thermal Losses During Hydrogen Manufacture for Coal Liquefaction

The calculation of thermal efficiency losses begins with the fact that almost all hydrogen used industrially is produced by partial oxidation and/or steam reforming of natural gas, petroleum fractions, or coal. Coal will be used more widely as petroleum and natural gas resources are depleted and hydrogen for coal liquefaction processes will be produced predominantly from coal.

The overall equation for hydrogen production from coal and oxygen is:



Let us assume that the coal liquefaction product is a liquid with a density of 7 lb/gallon (approx. 0.8g/ml).

1 bbl of product weighs 294 lbs.

To add 4 wt % hydrogen requires 12 lb H.

Using equation (a) above we can set up the following equation:

$$\frac{x}{13} = \frac{12}{1}$$

where the equated ratios are the weight of coal (or hydrogen) in pounds over the relative molecular weight of coal (CH) and hydrogen (H).

The result is that approximately 156 lbs. of coal is required to make enough hydrogen to produce 1 barrel of coal liquid.

Using the average yield of 2.5 barrels per ton of coal for the reductive processes and a four percent by weight hydrogen addition, we calculate 390 pounds of coal is needed to make the hydrogen. This amounts to approximately 16% loss in energy ($\frac{390}{2390}$). The precise loss of energy (coal) used for hydrogen will vary with process conditions and severity and these factors are considered in the range of energy losses due to hydrogen production given in the text.

The NRL process uses much less hydrogen than any reducing process. The hydrogen consumption of the NRL process can be calculated on the following basis:

Assume that the compounds identified by mass spectroscopy are representative and that they are formed by decarboxylation of the corresponding acids:



RCO_2H are the acids of the aromatics shown above in Appendix I.A. Average molecular weights of our products are approximately 200. If one hydrogen atom is required for each molecule, this would be $\frac{1}{200}$ or 0.5% by weight hydrogen. However, since an atom of hydrogen is produced during decarboxylation (H^* in equation (b) above), the actual hydrogen consumption is much less than 0.5%. We estimate that hydrogen consumption is approximately 0.2% by weight, or about 1/20 of the hydrogen requirement for reducing liquefaction processes.